

# (E)-[2-(1,3-Dithiolan-2-ylidene)-hydrazinylidene](3-fluorophenyl)methyl 3-fluorobenzoate

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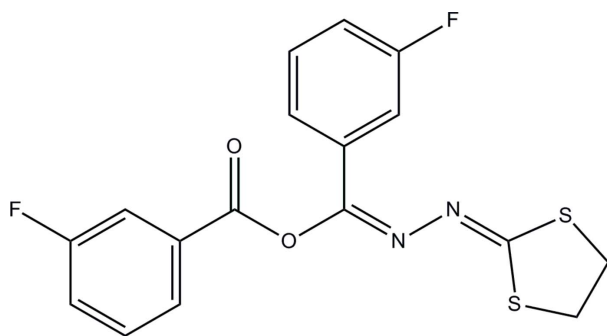
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Key indicators: single-crystal X-ray study;  $T = 113$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.031;  $wR$  factor = 0.076; data-to-parameter ratio = 12.8.

In the title compound,  $\text{C}_{17}\text{H}_{12}\text{F}_2\text{N}_2\text{O}_2\text{S}_2$ , the conformation of the dithiacyclopentane ring is a half-chair, with a total puckering amplitude  $Q_T = 0.460$  (1) Å.  $\pi$ - $\pi$  interactions [centroid-centroid distance = 3.585 (9) Å between the fluorophenyl rings of neighbouring molecules] and  $\text{C}-\text{H}\cdots\text{N}$  and  $\text{C}-\text{H}\cdots\text{O}$  interactions help to stabilize the crystal structure and form ladders along the  $c$  axis.

## Related literature

For the use of dithiolan heterocyclic compounds as broad-spectrum fungicides, see: Tanaka *et al.* (1976); Wang *et al.* (1994).



## Experimental

### Crystal data

$\text{C}_{17}\text{H}_{12}\text{F}_2\text{N}_2\text{O}_2\text{S}_2$   
 $M_r = 378.41$   
Triclinic,  $P\bar{1}$   
 $a = 9.124$  (4) Å  
 $b = 9.757$  (4) Å  
 $c = 10.738$  (4) Å  
 $\alpha = 104.592$  (3)°  
 $\beta = 110.326$  (5)°  
 $\gamma = 101.194$  (4)°  
 $V = 824.6$  (6) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.36$  mm<sup>-1</sup>  
 $T = 113$  K  
 $0.20 \times 0.20 \times 0.20$  mm

### Data collection

Rigaku Saturn724 CCD diffractometer  
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MS, 2009)  
 $T_{\min} = 0.932$ ,  $T_{\max} = 0.932$   
7057 measured reflections  
2896 independent reflections  
2098 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.036$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.076$   
 $S = 0.96$   
2896 reflections  
226 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.39$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.20$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C9}-\text{H9B}\cdots\text{O2}^{\text{i}}$	0.97	2.49	3.280 (2)	138
$\text{C10}-\text{H10B}\cdots\text{O2}^{\text{ii}}$	0.97	2.46	3.248 (2)	138
$\text{C13}-\text{H13A}\cdots\text{N1}^{\text{iii}}$	0.93	2.50	3.424 (3)	176

Symmetry codes: (i)  $-x, -y + 2, -z + 1$ ; (ii)  $x + 1, y, z$ ; (iii)  $-x, -y + 2, -z + 2$ .

Data collection: *CrystalClear-SM Expert* (Rigaku/MS, 2009); cell refinement: *CrystalClear-SM Expert*; data reduction: *CrystalClear-SM Expert*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5300).

## References

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Tanaka, H., Araki, F., Harada, T. & Kurono, H. (1976). Jpn Patent No. 51151326A.  
Wang, Y., Li, Z. H. & Gao, N. (1994). *Yaoxue Xuebao*, **29**, 78–80.

## supplementary materials

*Acta Cryst.* (2013). E69, o571 [doi:10.1107/S1600536813007319]

**(*E*)-[2-(1,3-Dithiolan-2-ylidene)hydrazinylidene](3-fluorophenyl)methyl 3-fluorobenzoate**

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**Comment**

Many dithiolan heterocyclic compounds have been widely used as potent and broad-spectrum fungicides (Tanaka *et al.*, 1976; Wang *et al.*, 1994). In order to search for new heterocyclic compounds with higher biological activities, we synthesized the (*E*)-((1,3-dithiolan-2-yl)diazanyl)(3-fluorophenyl)methyl 3-fluorobenzoate and describe its structure here.

In the title compound, C<sub>17</sub>H<sub>12</sub>F<sub>2</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>, the conformation of the dithiacyclopentane ring (C8—C10/S1—S2) is halfchair, with a total puckering amplitude  $Q_T = 0.460$  (1) Å.  $\pi$ - $\pi$  interactions (centroid-to-centroid distances 3.585 (9) Å between the fluorophenyl rings (C12—C17) of neighbouring molecules) and intermolecular C—H $\cdots$ N and C—H $\cdots$ O interactions help to stabilize the crystal structure (Table 1).

**Experimental**

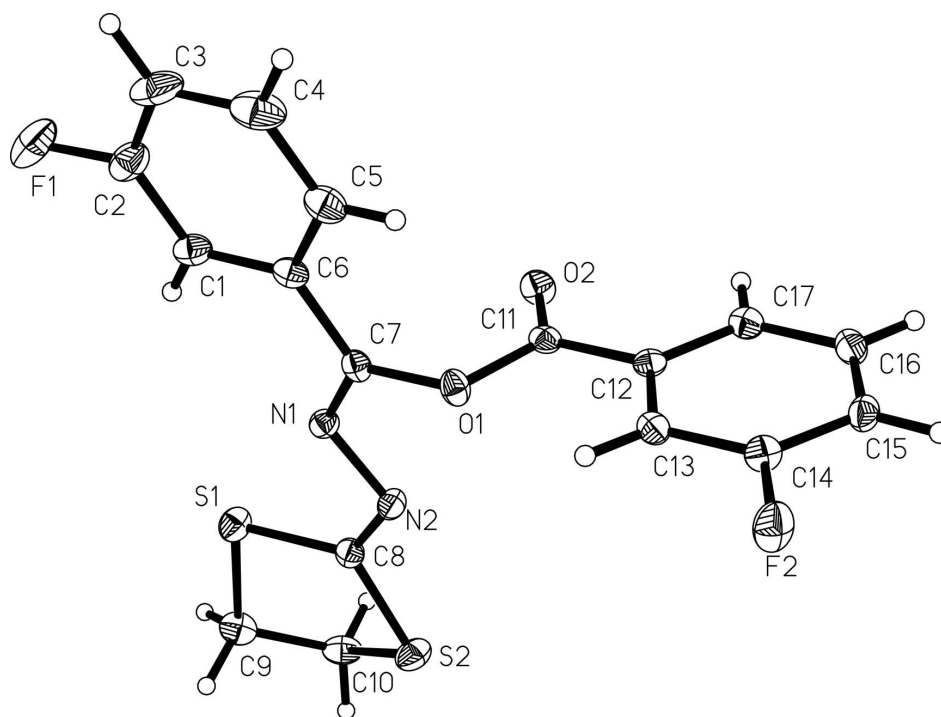
1.34 g (10 mmol) of (1,3-dithiolan-2-ylidene)hydrazine and 20 mmol triethylamine was dissolved in 15 ml of dichloromethane and stirred at room temperature, 3.17 g (20 mmol) 3-fluorobenzoyl chloride was added dropwise to the mixture. The reaction mixture was stirred vigorously at 273 K for 3 h. The reaction mixture was poured into 200 ml of water and extracted with three 50-ml portions of dichloromethane. The combined extracts were washed with saturated brine, dried over anhydrous sodium sulfate and evaporated on a rotary evaporator to afford the crude product, which was purified by column chromatography to yield the pure product as colorless crystals. Single crystals suitable for X-ray diffraction were obtained through slow evaporation of a solution of the pure title compound in ethanol.

**Refinement**

All H atoms bonded on carbon were found on difference maps, with C—H = 0.93 or 0.97 Å, and included in the final cycles of refinement using a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

**Computing details**

Data collection: *CrystalClear-SM Expert* (Rigaku/MS, 2009); cell refinement: *CrystalClear-SM Expert* (Rigaku/MS, 2009); data reduction: *CrystalClear-SM Expert* (Rigaku/MS, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

**Figure 1**

View of the title compound showing the atomic numbering and 40% probability displacement ellipsoids.

**(*E*)-[2-(1,3-Dithiolan-2-ylidene)hydrazinylidene](3-fluorophenyl)methyl 3-fluorobenzoate**

*Crystal data*

$C_{17}H_{12}F_2N_2O_2S_2$

$M_r = 378.41$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 9.124\ (4)\ \text{\AA}$

$b = 9.757\ (4)\ \text{\AA}$

$c = 10.738\ (4)\ \text{\AA}$

$\alpha = 104.592\ (3)^\circ$

$\beta = 110.326\ (5)^\circ$

$\gamma = 101.194\ (4)^\circ$

$V = 824.6\ (6)\ \text{\AA}^3$

$Z = 2$

$F(000) = 388$

$D_x = 1.524\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2617 reflections

$\theta = 2.2\text{--}27.9^\circ$

$\mu = 0.36\ \text{mm}^{-1}$

$T = 113\ \text{K}$

Block, colorless

$0.20 \times 0.20 \times 0.20\ \text{mm}$

*Data collection*

Rigaku Saturn724 CCD

diffractometer

Radiation source: rotating anode

Multilayer monochromator

Detector resolution:  $14.22\ \text{pixels mm}^{-1}$

$\omega$  and  $\varphi$  scans

Absorption correction: multi-scan

(*CrystalClear*; Rigaku/MS, 2009)

$T_{\min} = 0.932$ ,  $T_{\max} = 0.932$

7057 measured reflections

2896 independent reflections

2098 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 2.2^\circ$

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -12 \rightarrow 12$

# Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.031$ 
 $wR(F^2) = 0.076$ 
 $S = 0.96$ 

2896 reflections

226 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0322P)^2]$ 

where  $P = (F_o^2 + 2F_c^2)/3$ 
 $(\Delta/\sigma)_{\max} = 0.001$ 
 $\Delta\rho_{\max} = 0.39 \text{ e } \text{\AA}^{-3}$ 
 $\Delta\rho_{\min} = -0.20 \text{ e } \text{\AA}^{-3}$ 

# Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

# Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.10124 (6)	0.83442 (5)	0.59445 (5)	0.02517 (15)
O1	−0.12238 (14)	1.08666 (13)	0.92674 (12)	0.0209 (3)
N1	−0.06721 (17)	0.92577 (15)	0.75780 (14)	0.0183 (4)
F1	−0.49133 (14)	0.43408 (13)	0.61224 (12)	0.0447 (4)
C1	−0.3309 (2)	0.6858 (2)	0.71390 (18)	0.0234 (5)
H1B	−0.2714	0.6668	0.6602	0.028*
S2	0.31536 (6)	1.14801 (5)	0.73274 (5)	0.02773 (15)
F2	0.06577 (13)	1.50851 (11)	1.36811 (11)	0.0320 (3)
O2	−0.27848 (15)	1.15266 (14)	0.75200 (12)	0.0241 (3)
N2	0.05995 (17)	1.05067 (16)	0.78311 (15)	0.0205 (4)
C2	−0.4583 (2)	0.5746 (2)	0.7016 (2)	0.0300 (5)
C3	−0.5519 (2)	0.5965 (2)	0.7762 (2)	0.0378 (6)
H3A	−0.6389	0.5187	0.7637	0.045*
C4	−0.5130 (2)	0.7376 (3)	0.8706 (2)	0.0375 (6)
H4A	−0.5742	0.7552	0.9231	0.045*
C5	−0.3846 (2)	0.8530 (2)	0.88806 (19)	0.0277 (5)
H5A	−0.3591	0.9474	0.9524	0.033*
C6	−0.2929 (2)	0.8280 (2)	0.80908 (18)	0.0194 (4)
C7	−0.1555 (2)	0.94860 (19)	0.82551 (17)	0.0177 (4)
C8	0.1433 (2)	1.01277 (19)	0.71174 (18)	0.0196 (4)
C9	0.2838 (2)	0.8807 (2)	0.56131 (19)	0.0281 (5)
H9A	0.3748	0.8649	0.6302	0.034*
H9B	0.2634	0.8176	0.4675	0.034*
C10	0.3251 (2)	1.0425 (2)	0.57270 (19)	0.0273 (5)
H10A	0.2471	1.0544	0.4909	0.033*
H10B	0.4345	1.0771	0.5771	0.033*

C11	−0.1953 (2)	1.18274 (19)	0.87559 (19)	0.0183 (4)
C12	−0.1586 (2)	1.32341 (19)	0.99052 (18)	0.0176 (4)
C13	−0.0640 (2)	1.3463 (2)	1.13176 (18)	0.0193 (4)
H13A	−0.0256	1.2719	1.1584	0.023*
C14	−0.0294 (2)	1.4828 (2)	1.23034 (18)	0.0214 (4)
C15	−0.0852 (2)	1.5955 (2)	1.19552 (19)	0.0219 (4)
H15A	−0.0584	1.6869	1.2650	0.026*
C16	−0.1816 (2)	1.5698 (2)	1.05533 (19)	0.0235 (5)
H16A	−0.2215	1.6441	1.0299	0.028*
C17	−0.2192 (2)	1.4342 (2)	0.95261 (19)	0.0211 (4)
H17A	−0.2847	1.4171	0.8584	0.025*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0288 (3)	0.0228 (3)	0.0234 (3)	0.0054 (2)	0.0145 (2)	0.0038 (2)
O1	0.0265 (7)	0.0204 (7)	0.0161 (7)	0.0112 (6)	0.0082 (6)	0.0048 (6)
N1	0.0181 (8)	0.0184 (8)	0.0171 (8)	0.0044 (7)	0.0065 (7)	0.0062 (7)
F1	0.0460 (8)	0.0304 (7)	0.0372 (7)	−0.0090 (6)	0.0073 (6)	0.0089 (6)
C1	0.0196 (10)	0.0296 (11)	0.0191 (10)	0.0050 (9)	0.0059 (9)	0.0106 (9)
S2	0.0240 (3)	0.0262 (3)	0.0290 (3)	0.0009 (2)	0.0132 (2)	0.0055 (2)
F2	0.0423 (7)	0.0278 (6)	0.0184 (6)	0.0112 (5)	0.0067 (5)	0.0041 (5)
O2	0.0255 (7)	0.0278 (7)	0.0168 (7)	0.0102 (6)	0.0054 (6)	0.0076 (6)
N2	0.0213 (9)	0.0163 (8)	0.0221 (8)	0.0036 (7)	0.0093 (7)	0.0052 (7)
C2	0.0285 (12)	0.0274 (11)	0.0230 (11)	0.0003 (9)	0.0028 (10)	0.0088 (10)
C3	0.0219 (12)	0.0488 (15)	0.0404 (13)	−0.0011 (11)	0.0090 (11)	0.0265 (12)
C4	0.0287 (12)	0.0591 (16)	0.0381 (13)	0.0155 (11)	0.0211 (11)	0.0265 (12)
C5	0.0259 (11)	0.0374 (12)	0.0253 (11)	0.0146 (10)	0.0111 (10)	0.0156 (10)
C6	0.0178 (10)	0.0271 (11)	0.0146 (10)	0.0087 (8)	0.0051 (8)	0.0101 (9)
C7	0.0204 (10)	0.0196 (10)	0.0119 (9)	0.0090 (8)	0.0040 (8)	0.0056 (8)
C8	0.0211 (10)	0.0195 (10)	0.0166 (10)	0.0067 (8)	0.0050 (9)	0.0074 (8)
C9	0.0277 (12)	0.0366 (12)	0.0230 (11)	0.0118 (10)	0.0136 (10)	0.0092 (10)
C10	0.0207 (10)	0.0397 (12)	0.0225 (11)	0.0069 (9)	0.0100 (9)	0.0130 (10)
C11	0.0157 (10)	0.0218 (10)	0.0224 (11)	0.0063 (8)	0.0110 (9)	0.0111 (9)
C12	0.0149 (10)	0.0203 (10)	0.0200 (10)	0.0037 (8)	0.0102 (8)	0.0080 (8)
C13	0.0195 (10)	0.0205 (10)	0.0227 (10)	0.0079 (8)	0.0110 (9)	0.0106 (9)
C14	0.0228 (11)	0.0244 (11)	0.0169 (10)	0.0065 (9)	0.0090 (9)	0.0065 (9)
C15	0.0238 (11)	0.0172 (10)	0.0254 (11)	0.0050 (8)	0.0141 (9)	0.0041 (9)
C16	0.0245 (11)	0.0217 (10)	0.0301 (11)	0.0103 (9)	0.0150 (10)	0.0110 (9)
C17	0.0204 (10)	0.0242 (10)	0.0222 (10)	0.0073 (8)	0.0102 (9)	0.0114 (9)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

S1—C8	1.7499 (19)	C5—C6	1.395 (2)
S1—C9	1.8178 (18)	C5—H5A	0.9300
O1—C11	1.368 (2)	C6—C7	1.469 (2)
O1—C7	1.401 (2)	C9—C10	1.513 (3)
N1—C7	1.274 (2)	C9—H9A	0.9700
N1—N2	1.4036 (19)	C9—H9B	0.9700
F1—C2	1.366 (2)	C10—H10A	0.9700

C1—C2	1.370 (2)	C10—H10B	0.9700
C1—C6	1.394 (2)	C11—C12	1.483 (2)
C1—H1B	0.9300	C12—C17	1.392 (3)
S2—C8	1.7480 (18)	C12—C13	1.393 (2)
S2—C10	1.8088 (19)	C13—C14	1.374 (2)
F2—C14	1.357 (2)	C13—H13A	0.9300
O2—C11	1.200 (2)	C14—C15	1.378 (3)
N2—C8	1.294 (2)	C15—C16	1.381 (2)
C2—C3	1.370 (3)	C15—H15A	0.9300
C3—C4	1.381 (3)	C16—C17	1.382 (2)
C3—H3A	0.9300	C16—H16A	0.9300
C4—C5	1.380 (3)	C17—H17A	0.9300
C4—H4A	0.9300		
C8—S1—C9	95.19 (8)	S1—C9—H9A	110.1
C11—O1—C7	115.41 (14)	C10—C9—H9B	110.1
C7—N1—N2	115.89 (14)	S1—C9—H9B	110.1
C2—C1—C6	118.25 (17)	H9A—C9—H9B	108.4
C2—C1—H1B	120.9	C9—C10—S2	107.36 (12)
C6—C1—H1B	120.9	C9—C10—H10A	110.2
C8—S2—C10	94.44 (8)	S2—C10—H10A	110.2
C8—N2—N1	110.12 (14)	C9—C10—H10B	110.2
F1—C2—C1	118.15 (17)	S2—C10—H10B	110.2
F1—C2—C3	118.45 (17)	H10A—C10—H10B	108.5
C1—C2—C3	123.39 (19)	O2—C11—O1	122.43 (17)
C2—C3—C4	117.95 (18)	O2—C11—C12	125.87 (18)
C2—C3—H3A	121.0	O1—C11—C12	111.70 (15)
C4—C3—H3A	121.0	C17—C12—C13	120.61 (17)
C5—C4—C3	120.84 (18)	C17—C12—C11	117.79 (17)
C5—C4—H4A	119.6	C13—C12—C11	121.59 (18)
C3—C4—H4A	119.6	C14—C13—C12	117.59 (18)
C4—C5—C6	119.96 (18)	C14—C13—H13A	121.2
C4—C5—H5A	120.0	C12—C13—H13A	121.2
C6—C5—H5A	120.0	F2—C14—C13	118.49 (18)
C1—C6—C5	119.59 (17)	F2—C14—C15	118.47 (16)
C1—C6—C7	119.26 (15)	C13—C14—C15	123.03 (18)
C5—C6—C7	121.15 (16)	C14—C15—C16	118.59 (17)
N1—C7—O1	122.72 (15)	C14—C15—H15A	120.7
N1—C7—C6	121.68 (16)	C16—C15—H15A	120.7
O1—C7—C6	115.47 (14)	C15—C16—C17	120.32 (19)
N2—C8—S2	118.67 (14)	C15—C16—H16A	119.8
N2—C8—S1	125.76 (13)	C17—C16—H16A	119.8
S2—C8—S1	115.57 (10)	C16—C17—C12	119.84 (18)
C10—C9—S1	108.17 (13)	C16—C17—H17A	120.1
C10—C9—H9A	110.1	C12—C17—H17A	120.1
C7—N1—N2—C8	178.22 (16)	C10—S2—C8—S1	17.80 (12)
C6—C1—C2—F1	−177.56 (17)	C9—S1—C8—N2	−174.67 (17)
C6—C1—C2—C3	1.1 (3)	C9—S1—C8—S2	4.65 (12)

F1—C2—C3—C4	177.36 (18)	C8—S1—C9—C10	−31.34 (14)
C1—C2—C3—C4	−1.3 (3)	S1—C9—C10—S2	46.97 (15)
C2—C3—C4—C5	0.5 (3)	C8—S2—C10—C9	−38.84 (15)
C3—C4—C5—C6	0.4 (3)	C7—O1—C11—O2	−1.9 (2)
C2—C1—C6—C5	−0.1 (3)	C7—O1—C11—C12	177.88 (12)
C2—C1—C6—C7	179.21 (16)	O2—C11—C12—C17	−3.1 (3)
C4—C5—C6—C1	−0.6 (3)	O1—C11—C12—C17	177.18 (14)
C4—C5—C6—C7	−179.95 (17)	O2—C11—C12—C13	178.22 (16)
N2—N1—C7—O1	−4.3 (2)	O1—C11—C12—C13	−1.5 (2)
N2—N1—C7—C6	179.92 (15)	C17—C12—C13—C14	−1.8 (2)
C11—O1—C7—N1	89.6 (2)	C11—C12—C13—C14	176.82 (14)
C11—O1—C7—C6	−94.45 (18)	C12—C13—C14—F2	−178.49 (14)
C1—C6—C7—N1	−1.9 (3)	C12—C13—C14—C15	0.6 (3)
C5—C6—C7—N1	177.38 (17)	F2—C14—C15—C16	179.79 (15)
C1—C6—C7—O1	−177.96 (16)	C13—C14—C15—C16	0.7 (3)
C5—C6—C7—O1	1.4 (2)	C14—C15—C16—C17	−0.8 (3)
N1—N2—C8—S2	−176.83 (12)	C15—C16—C17—C12	−0.4 (3)
N1—N2—C8—S1	2.5 (2)	C13—C12—C17—C16	1.8 (2)
C10—S2—C8—N2	−162.83 (16)	C11—C12—C17—C16	−176.95 (15)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C9—H9 <i>B</i> $\cdots$ O2 <sup>i</sup>	0.97	2.49	3.280 (2)	138
C10—H10 <i>B</i> $\cdots$ O2 <sup>ii</sup>	0.97	2.46	3.248 (2)	138
C13—H13 <i>A</i> $\cdots$ N1 <sup>iii</sup>	0.93	2.50	3.424 (3)	176

Symmetry codes: (i)  $-x, -y+2, -z+1$ ; (ii)  $x+1, y, z$ ; (iii)  $-x, -y+2, -z+2$ .